

CLAIMS

1. A method of forming a thin film on a base substance via an intermediate layer, comprising the steps of:

5 calculating an interface energy E_a at an interface A between said base substance and said intermediate layer and an interface energy E_b at an interface B between said intermediate layer and said thin film;

calculating an interface energy E_c at an interface C between said base substance and said thin film in a state where said intermediate layer is omitted; and

10 selecting a substance for said intermediate layer so as to satisfy conditions of $E_a < E_c$ and $E_b < E_c$.

2. The thin film forming method according to claim 1, wherein each of said interface energies E_a and E_b is lower than 2 J/m^2 .

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3. The thin film forming method according to claim 1, wherein after calculating an energy E_d of a crystal including the interface and an energy E_p of a perfect crystal taking account of chemical potentials of constituent elements by the first-principles calculation band method, each of said interface energies E_a , E_b and E_c is calculated as $E_d - E_p$.

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4. The thin film forming method according to claim 1, wherein in at least one of said interfaces A and B, substances on both sides of the interface share a specific atomic layer contained in common therein, to thereby reduce the interface energy.

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5. The thin film forming method according to claim 1, wherein at least one of said interfaces A and B has a small difference in crystal lattice constant compared to said interface C, to thereby reduce the interface energy.

6. The thin film forming method according to claim 1, wherein said substance for said intermediate layer is an oxide having a stacked-layer structure containing at least two kinds of atomic layers, wherein one kind of said atomic layers decreases said interface energy E_a compared to said interface energy E_c , and another kind of said atomic layers decreases said interface energy E_b compared to said interface energy E_c .

7. The thin film forming method according to claim 1, wherein said substance for said intermediate layer has a crystal structure of a perovskite type.

8. The thin film forming method according to claim 6, wherein, when said oxide as said substance for said intermediate layer includes a coordination polyhedron formed of oxygen ions surrounding a metal ion, in at least one of said interfaces A and B, the oxygen ions are also linked with another substance constituting the interface.

9. The thin film forming method according to claim 6, wherein said base substance has a crystal structure of a rock-salt type.

10. The thin film forming method according to claim 1, wherein said base substance is MgO , said substance for said intermediate layer is $BaZrO_3$, and said thin film is $RE_{1+x}Ba_{2-x}Cu_3O_{7-y}$ where RE represents at least one kind of rare earth elements.